Application Readiness at NERSC

IXPUG 2016
Argonne National Lab
Sep. 20, 2016

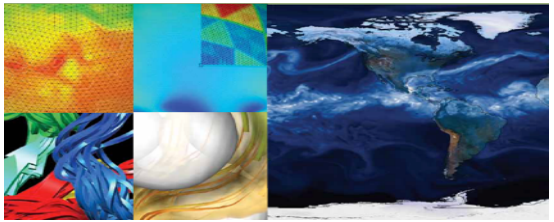
Richard Gerber

Senior Science Advisor
HPC Department Head (Acting)

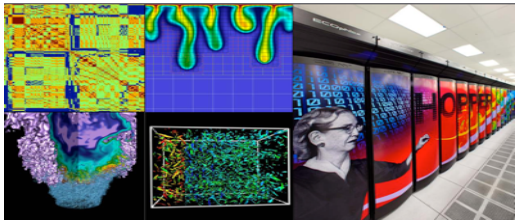
NERSC: the Mission HPC Facility for DOE Office of Science Research

U.S. DEPARTMENT OF ENERGY | Office of Science

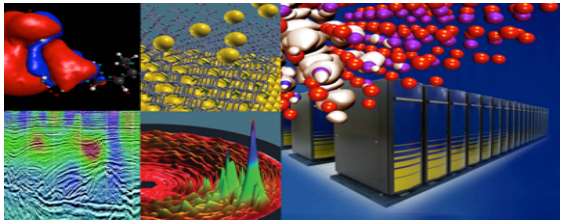
Largest funder of physical science research in U.S.



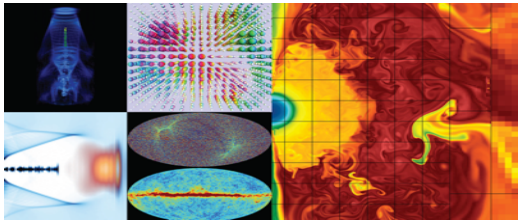
Bio Energy, Environment



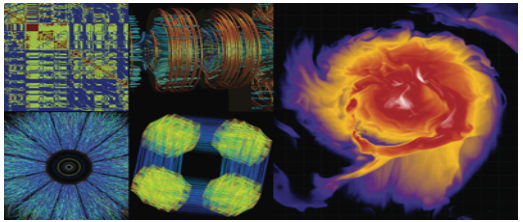
Computing



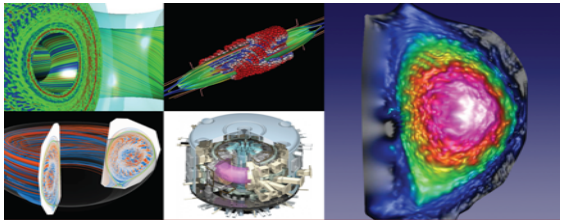
Materials, Chemistry, Geophysics



Particle Physics, Astrophysics



Nuclear Physics



Fusion Energy, Plasma Physics

6,000 users, 48 states, 40 countries, universities & national labs

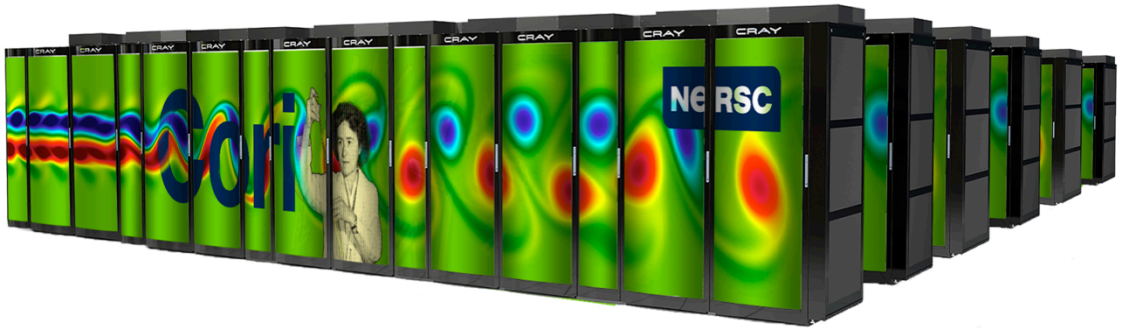
Current Production Systems

Edison

5,560 Ivy Bridge Nodes / 24 cores/node
133 K cores, 64 GB memory/node
Cray XC30 / Aries Dragonfly interconnect
6 PB Lustre Cray Sonexion scratch FS

Cori Phase 1

1,630 Haswell Nodes / 32 cores/node
52 K cores, 128 GB memory/node
Cray XC40 / Aries Dragonfly interconnect
24 PB Lustre Cray Sonexion scratch FS
1.5 PB Burst Buffer



Cori Phase 2 – Being installed now!

Cray XC40 system with 9,300 Intel Knights Landing compute nodes

68 cores / 96 GB DRAM / 16 GB HBM

Support the entire Office of Science research community

Begin to transition workload to energy efficient architectures

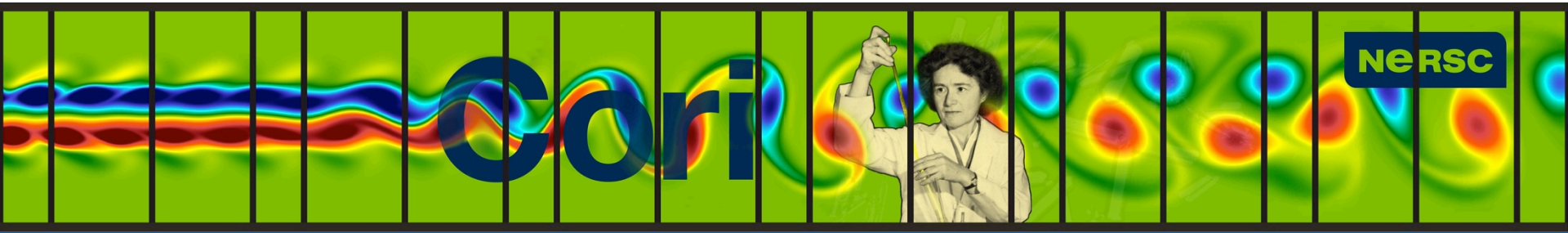
Data Intensive Science Support

10 Haswell processor cabinets (Phase 1)

NVRAM Burst Buffer 1.5 PB, 1.5 TB/sec

30 PB of disk, >700 GB/sec I/O bandwidth

Integrate with Cori Phase 1 on Aries network for data / simulation / analysis on one system



Gerty Cori

First American woman Nobel Prize winner, third ever, and first woman in Physiology & Medicine

… for the discovery of the mechanism by which glycogen–a derivative of glucose–is broken down in muscle tissue into lactic acid and then resynthesized in the body and stored as a source of energy

Edison, Hopper, Franklin, Bassi, Carver, Seaborg, Mcurie, Pierre, Jacquard, Bhaskara, Euclid, DaVinci, JWatson, FCrick, Kileen

Cori Integration Status

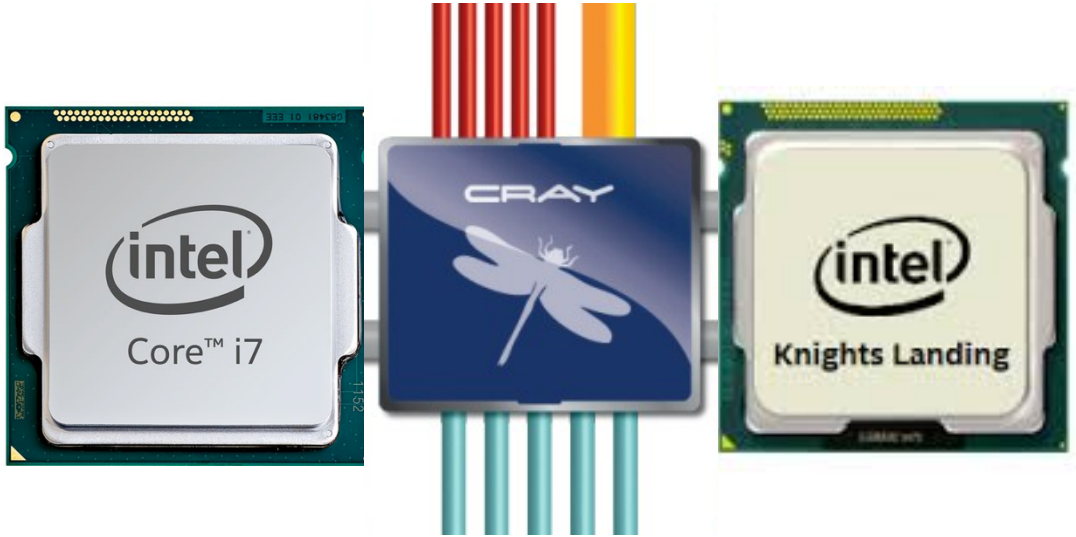
July-August
- 9300 KNL nodes arrive, installed, tested

Monday
- P1 shut down, P2 stress test

This week
- Move I/O, network blades
- Add Haswell to P1 to fill holes
- Cabling/Re-cabling
- Aries/LNET config
- Cabinet reconfigs

Now to now+6 weeks
- …continue, test, resolve issues
- configure SLURM

NESAP code team access ASAP!

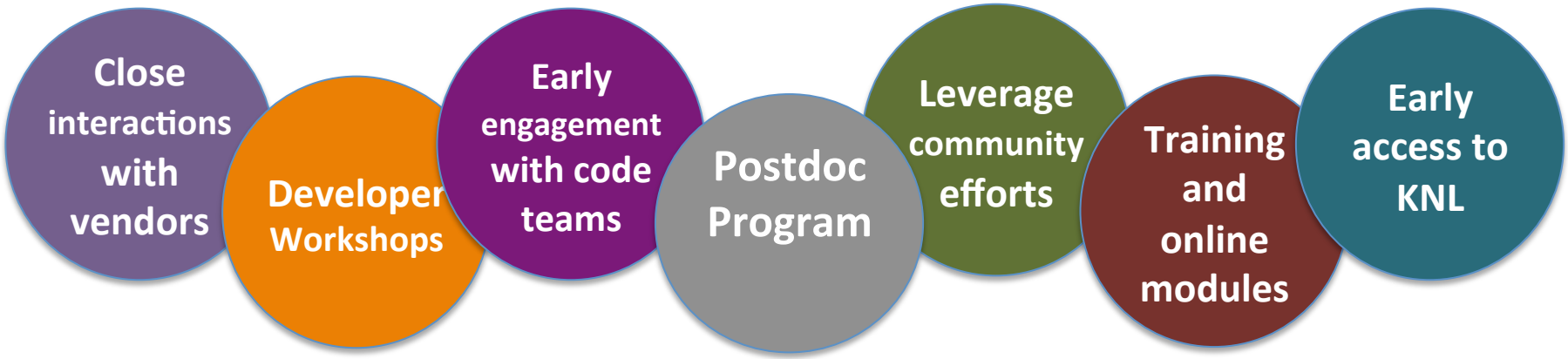


NERSC Exascale Scientific Application Program (NESAP)

Goal: Prepare DOE Office of Science users for many core

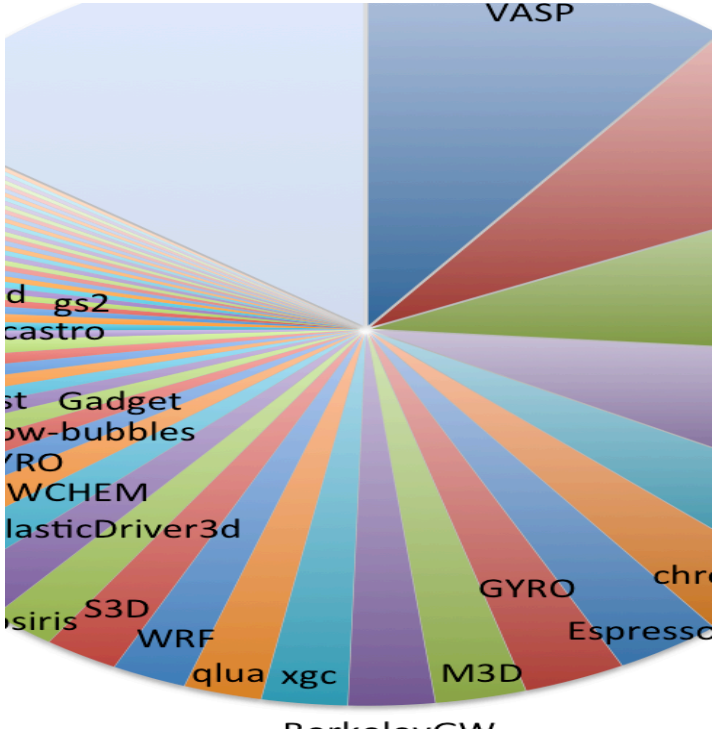
Partner closely with ~20 application teams and apply lessons learned to broad NERSC user community

NESAP activities include:



NESAP Focus on 20 codes

Application Hours at NERSC 2013



10 codes make up 50% of the workload

25 codes make up 66% of the workload

Edison will be available until 2019

Training and lessons learned will be made available to all application teams

Application Readiness

A few NERSC staff have been on Cori Phase 2 as stand-alone system, but with limited usability and access.

Just trying to get things to run; had some success, some failures.

NESAP team will get access once the system is integrated and checks out OK. ~Late October ???

Preparation and optimization work continues with NERSC/LBNL application readiness team, IXPUG, Cray, Intel, DOE labs

Details in Jack Deslippe's talk this afternoon!

NERSC NESAP Staff

Katie Antypas

Nick Wright

Richard Gerber

Brian Austin

Zhengji Zhao

Helen He

Stephen Leak

Woo-Sun Yang

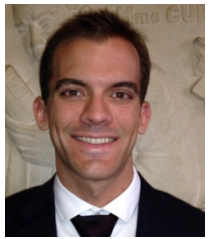
Rebecca Hartman-Baker

Doug Doerfler

Jack Deslippe

Brandon Cook

Thorsten Kurth


Brian Friesen

NESAP Postdocs

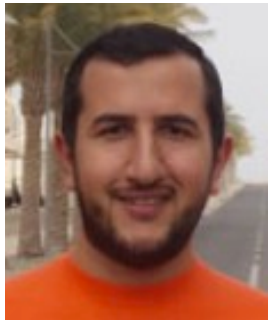
Taylor Barnes
Quantum ESPRESSO

Zahra
Ronaghi

Andrey Ovsyannikov
Chombo-Crunch

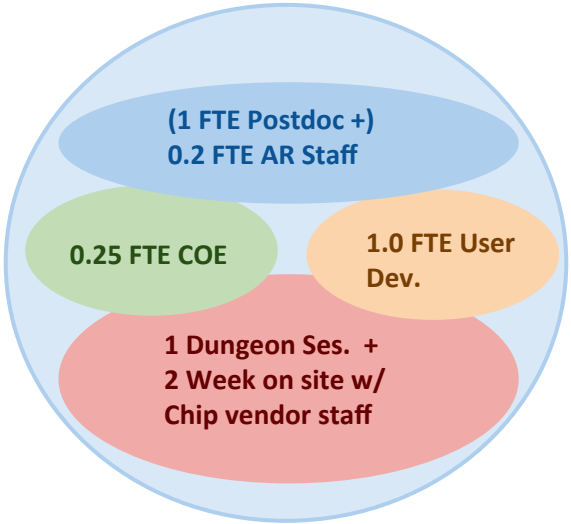
Mathieu Lobet
WARP

Tuomas Koskela
XGC1



Tareq Malas
EMGeo

Target Application Team Concept



Waiting for KNL …

We just can’t wait to get staff and users on Cori Phase 2!!!!

NERSC